(1,1'-Biphenyl)-2,2'-diol 1806-29-7 | DTXSID6051809

Model Performance

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Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 119 °C

Global applicability domain: Inside

Local applicability domain index: 8.24e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

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(1,1'-Biphenyl)-2,2'-diol

Measured: 109 Predicted: 119

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Biphenyl-2,5-diol Measured: 103 Predicted: 117

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1,4-Benzenediol, 2-(phenylmethyl)-Measured: 106 Predicted: 117

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Menadiol
Measured: 169
Predicted: 138

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4,4'-Propane-1,1-diyldiphenol

Measured: 132 Predicted: 133